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Supplymentary information

Synthesis and Characterization of Cobalt(III) Cyanide Complexes: Cobalt Participate in the Decomposition of Radical Anion of TCNQ

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Table S1. Selected bond lengths (Å) and angles (°) for **1**.

N(1)-Co(1)	1.892(3)	C(21)-Co(1)	1.932(4)
N(2)-Co(1)	1.894(3)	C(22)-Co(1)	1.941(4)
O(1)-Co(1)	1.916(3)	O(2)-Co(1)	1.911(3)
C(21)-K(1)#1	2.989(4)	O(2)-K(1)	2.709(3)
C(22)-K(1)	3.094(4)	O(2)-K(1)#1	3.333(3)
N(3)-K(1)#2	2.739(4)	K(1)-N(3)#3	2.739(4)
N(3)-K(1)#1	3.050(4)	K(1)-O(1)#4	2.788(3)
N(4)-K(1)	3.308(5)	K(1)-C(21)#4	2.989(4)
O(1)-K(1)#1	2.788(3)	K(1)-N(3)#4	3.050(4)
O(1)-K(1)	2.974(3)	K(1)-O(2)#4	3.333(3)
N(1)-Co(1)-O(2)	95.10(12)	N(2)-Co(1)-C(21)	88.95(15)
N(2)-Co(1)-O(2)	177.99(13)	O(2)-Co(1)-C(21)	89.57(15)
N(1)-Co(1)-O(1)	178.66(12)	O(1)-Co(1)-C(21)	91.41(14)
N(2)-Co(1)-O(1)	95.08(13)	N(1)-Co(1)-C(22)	90.30(15)
O(2)-Co(1)-O(1)	83.60(11)	N(2)-Co(1)-C(22)	89.63(15)
N(1)-Co(1)-C(21)	88.87(14)	O(2)-Co(1)-C(22)	91.86(14)
O(1)-Co(1)-C(22)	89.45(14)		

Symmetry transformations used to generate equivalent atoms:

#1 x, -y+3/2, z-1/2	#2 x, y, z-1	#3 x, y, z+1	#4 x, -y+3/2, z+1/2

Table S2. Selected bond lengths (Å) and angles (°) for **1S**.

Co(1)-N(1)	1.887(7)	Co(2)-N(3)	1.902(6)
Co(1)-N(2)	1.893(6)	Co(2)-N(4)	1.904(6)
Co(1)-C(21)	1.916(9)	Co(2)-O(4)	1.907(6)
Co(1)-O(2)	1.912(6)	Co(2)-O(3)	1.913(6)
Co(1)-O(1)	1.915(6)	Co(2)-C(44)	1.915(12)
Co(1)-C(22)	1.931(11)	Co(2)-C(45)	1.974(11)
K(2)-N(7)	2.647(11)	K(1)-C(21)	3.273(9)
K(2)-O(3)#4	2.793(8)	K(1)-O(2)#6	3.343(7)
K(2)-O(4)#4	2.791(7)	O(2)-K(1)#3	3.343(7)
K(2)-N(7)#5	2.950(10)	O(1)-K(1)#3	3.232(7)
K(2)-C(44)#5	3.011(9)	O(4)-K(2)#1	2.791(7)
K(2)-O(4)#5	3.150(7)	O(4)-K(2)#2	3.150(7)
K(2)-C(45)#4	3.226(8)	O(3)-K(2)#1	2.793(8)
K(2)-O(3)#5	3.338(8)	O(3)-K(2)#2	3.338(8)
K(1)-N(5)#4	2.699(11)	N(7)-K(2)#2	2.950(10)
K(1)-O(2)	2.732(7)	N(5)-K(1)#1	2.699(11)
K(1)-O(1)	2.834(8)	N(5)-K(1)#3	2.945(11)
K(1)-N(5)#6	2.945(11)	C(45)-K(2)#1	3.226(8)
K(1)-C(22)#6	2.998(9)	C(44)-K(2)#2	3.011(9)
K(1)-O(1W)	3.156(19)	C(22)-K(1)#3	2.998(9)
K(1)-O(1)#6	3.232(7)		
N(1)-Co(1)-N(2)	87.0(3)	N(3)-Co(2)-N(4)	85.5(3)
N(1)-Co(1)-C(21)	89.8(4)	N(3)-Co(2)-O(4)	179.1(3)
N(2)-Co(1)-C(21)	90.2(3)	N(4)-Co(2)-O(4)	95.3(2)
N(1)-Co(1)-O(2)	177.5(3)	N(3)-Co(2)-O(3)	96.2(3)
N(2)-Co(1)-O(2)	94.7(3)	N(4)-Co(2)-O(3)	176.8(3)
C(21)-Co(1)-O(2)	92.0(3)	O(4)-Co(2)-O(3)	83.0(2)
N(1)-Co(1)-O(1)	94.6(3)	N(3)-Co(2)-C(44)	89.7(4)
N(2)-Co(1)-O(1)	178.2(2)	N(4)-Co(2)-C(44)	86.9(4)
C(21)-Co(1)-O(1)	90.7(3)	O(4)-Co(2)-C(44)	90.7(4)
O(2)-Co(1)-O(1)	83.7(3)	O(3)-Co(2)-C(44)	90.4(4)
N(1)-Co(1)-C(22)	88.7(3)	N(3)-Co(2)-C(45)	88.7(3)
N(2)-Co(1)-C(22)	87.6(3)	N(4)-Co(2)-C(45)	92.3(3)
C(21)-Co(1)-C(22)	177.4(4)	O(4)-Co(2)-C(45)	90.9(3)
O(2)-Co(1)-C(22)	89.5(3)	O(3)-Co(2)-C(45)	90.5(3)
O(1)-Co(1)-C(22)	91.6(3)	C(44)-Co(2)-C(45)	178.3(4)

Symmetry transformations used to generate equivalent:

#1 x, y+1, z #2 -x+1, y+1/2, -z #3 -x+2, y+1/2, -z+1 #4 x, y-1, z

#5 -x+1, y-1/2, -z #6 -x+2, y-1/2, -z+1

Table S3. Selected bond lengths (Å) and angles (°) for **1R**.

Co(1)-N(1)	1.897(5)	Co(2)-N(3)	1.885(5)
Co(1)-O(1)	1.905(4)	Co(2)-N(4)	1.892(5)
Co(1)-O(2)	1.915(4)	Co(2)-O(3)	1.911(5)
Co(1)-N(2)	1.908(5)	Co(2)-C(44)	1.920(9)
Co(1)-C(22)	1.919(8)	Co(2)-O(4)	1.918(5)
Co(1)-C(21)	1.925(7)	Co(2)-C(45)	1.950(9)
K(1)-N(5)#1	2.720(8)	K(2)-C(45)#1	3.228(7)
K(1)-O(2)	2.748(5)	K(2)-O(4)#4	3.228(5)
K(1)-O(1)	2.841(5)	C(22)-K(1)#3	3.014(7)
K(1)-N(5)#2	2.992(8)	C(44)-K(2)#5	2.967(7)
K(1)-C(22)#2	3.014(7)	C(45)-K(2)#6	3.228(7)
K(1)-O(1)#2	3.040(5)	O(1)-K(1)#3	3.040(5)
K(1)-C(21)	3.280(7)	O(3)-K(2)#6	2.799(5)
K(2)-N(7)	2.678(8)	O(3)-K(2)#5	3.119(5)
K(2)-O(3)#1	2.799(5)	O(4)-K(2)#6	2.795(5)
K(2)-O(4)#1	2.795(5)	O(4)-K(2)#5	3.228(5)
K(2)-N(7)#4	2.942(8)	N(5)-K(1)#6	2.720(8)
K(2)-C(44)#4	2.967(7)	N(5)-K(1)#3	2.992(8)
K(2)-O(3)#4	3.119(5)	N(7)-K(2)#5	2.942(8)
N(1)-Co(1)-O(1)	95.2(2)	N(3)-Co(2)-N(4)	86.1(2)
N(1)-Co(1)-O(2)	178.0(2)	N(3)-Co(2)-O(3)	176.8(2)
O(1)-Co(1)-O(2)	83.98(19)	N(4)-Co(2)-O(3)	95.6(2)
N(1)-Co(1)-N(2)	86.2(2)	N(3)-Co(2)-C(44)	87.2(3)
O(1)-Co(1)-N(2)	177.4(2)	N(4)-Co(2)-C(44)	91.0(3)
O(2)-Co(1)-N(2)	94.5(2)	O(3)-Co(2)-C(44)	90.1(3)
N(1)-Co(1)-C(22)	87.9(3)	N(3)-Co(2)-O(4)	96.1(2)
O(1)-Co(1)-C(22)	90.6(3)	N(4)-Co(2)-O(4)	177.2(2)
O(2)-Co(1)-C(22)	90.2(3)	O(3)-Co(2)-O(4)	82.22(19)
N(2)-Co(1)-C(22)	87.3(3)	C(44)-Co(2)-O(4)	90.7(3)
N(1)-Co(1)-C(21)	90.3(3)	N(3)-Co(2)-C(45)	92.8(3)
O(1)-Co(1)-C(21)	91.3(2)	N(4)-Co(2)-C(45)	86.5(3)
O(2)-Co(1)-C(21)	91.6(3)	O(3)-Co(2)-C(45)	89.9(3)
N(2)-Co(1)-C(21)	90.8(3)	C(44)-Co(2)-C(45)	177.5(3)
C(22)-Co(1)-C(21)	177.5(3)	O(4)-Co(2)-C(45)	91.7(3)

Symmetry transformations used to generate equivalent atoms:

#1 x, y+1, z #2 -x, y+1/2, -z+1 #3 -x, y-1/2, -z+1 #4 -x+1, y+1/2, -z+2 #5 -x+1, y-1/2, -z+2 #6 x, y-1, z

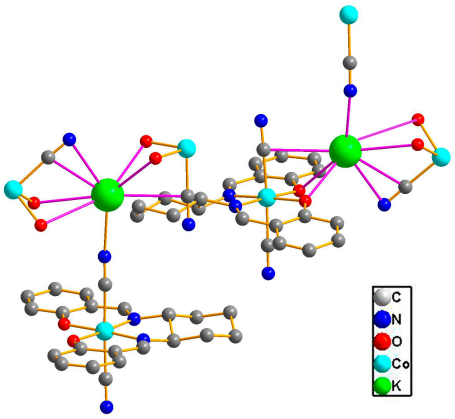


Figure S1. Asymmetric unit of complex **1R,** with some additional symmetry-equivalent atoms included to complete the coordination spheres around the metal atoms.

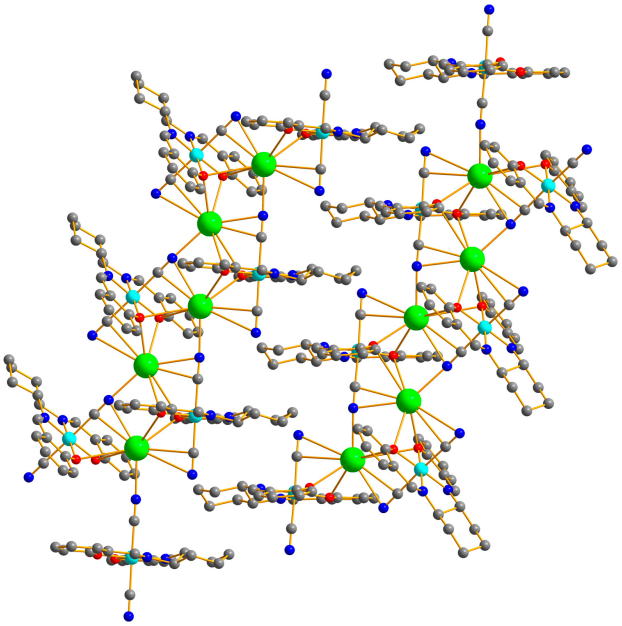
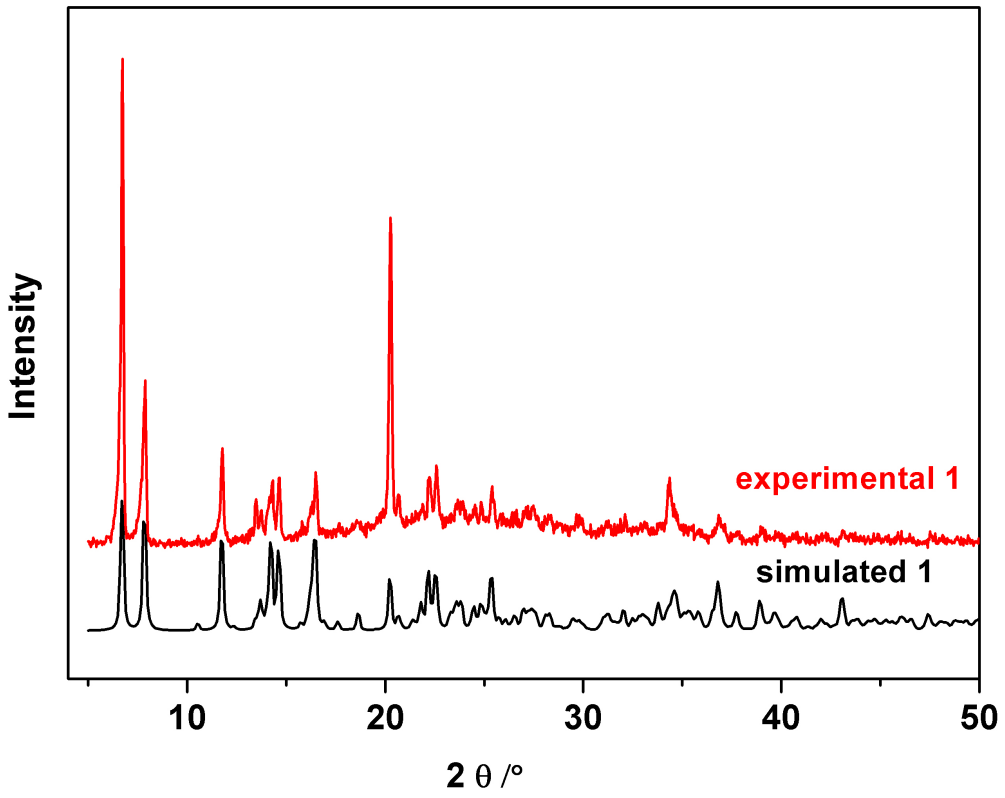
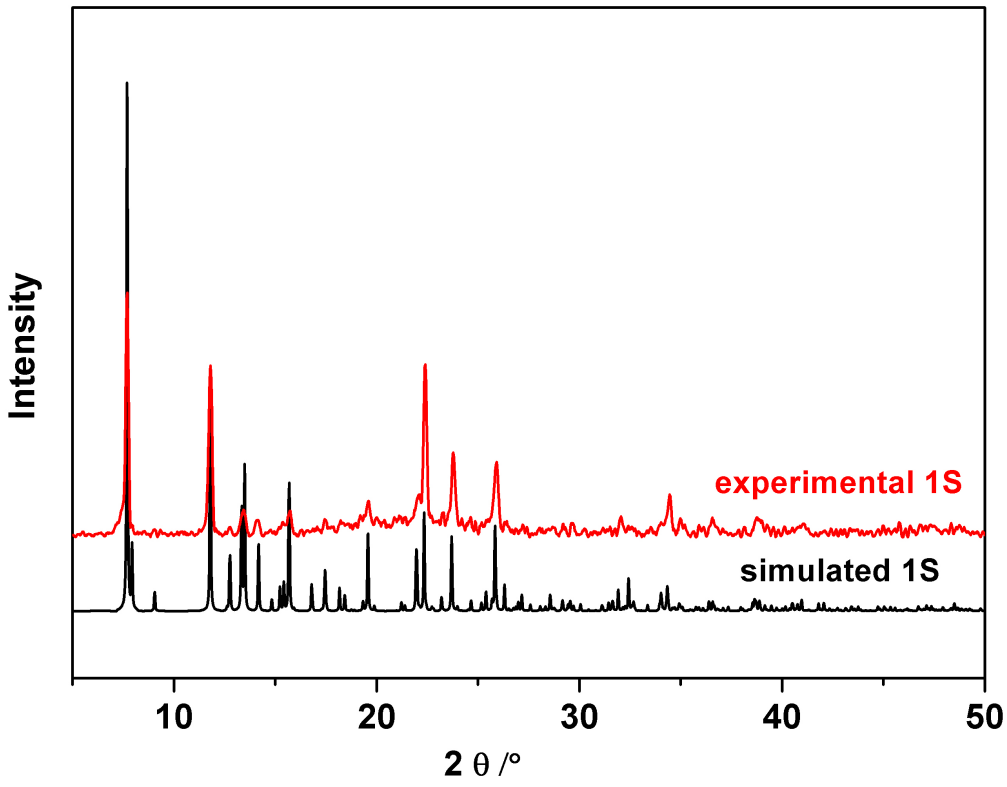


Figure S2 view of coordination chain in complex **1R** (Ni turquoise, K green, O red, N blue, C gray).





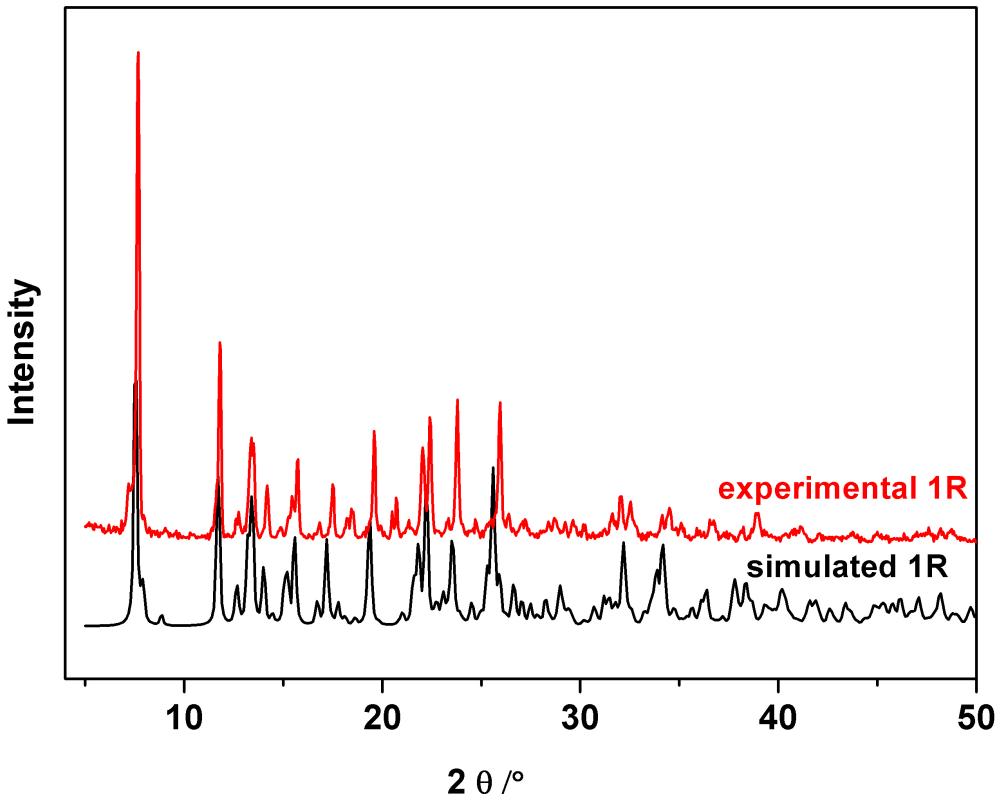


Figure S3. The experimental and simulated powder XRD diagrams of **1**, **1S** and **1R**.

Notes: The experimental powdered X-ray diffraction patterns of **1**, **1S** and **1R** agree well with the simulated ones based on the single-crystal X-ray data, indicating that they are in a pure phase.